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(December 4, 2001)

We study the violations of Bell inequality and reduction criteria for thermal states of qubits in a multi-qubit Heisenberg model as a function of temperature and external magnetic fields. Unlike the behaviors of the entanglement the violations can not be obtained by increasing the temperature or the magnetic field. The critical temperatures of the violations are found be less than that of the entanglement. We also consider a realistic cavity-QED model which is a special case of the multi-qubit Heisenberg model.

PACS numbers: 03.65.Ud, 03.67.-a, 75.50.Ee

Historically the violation of Bell inequalities [1] was considered as a means of determining whether there is entanglement between two qubits. In 1989 Werner [2] demonstrated that there exists states which are entangled but do not violate any Bell-type inequality, i.e., not all entangled states violate a Bell inequality. Further studies [3,4] showed that the maximal violation of a Bell inequality does not behave monotonously under local operation and classical communications. So Bell violations only give a hint for entanglement and can be considered an entanglement witness [5]. Most recently Scarani and Gisin built the relations between Bell inequalities and the usefulness for quantum key distribution [6] and quantum secret sharing [7], and Dür showed that even multipartite bound entangled states can violate Bell inequalities [8].

An interesting and natural type of entanglement, thermal entanglement, was introduced in magnetic systems and studied within the Heisenberg isotropic [9], anisotropic Heisenberg models [10,11] and the Ising model in a magnetic field [12]. Another natural type of entanglement was recently introduced in Bose-Einstein condensates [13]. The Gibbs state of a system at thermodynamic equilibrium is represented by the density operator

$$\rho(T) = \exp(-H/kT)/Z, \quad (1)$$

where $Z = \text{tr}[\exp(-H/kT)]$ is the partition function, H the system Hamiltonian, k is Boltzmann's constant which we henceforth take equal to 1, and $T = 1/\beta$ the temperature. As $\rho(T)$ represents a thermal state, the entanglement in the state is called *thermal entanglement* [9]. At $T = 0$, $\rho(T)$ represents the ground state which is pure for the non-degenerate case and mixed for the degenerate case. The ground state can be entangled but the thermal state $\rho(T)$ at $T = \infty$ can not be entangled as $\rho(T)$ is a completely random mixture. The entanglement in the ground state of isotropic Heisenberg models was studied in the literature [14,15]. A recent interesting work [16] showed that the success of the density matrix renormalization group method in understanding quantum phase transitions [17] is due to the way it preserves quantum entanglement under renormalization.

A complication in the analysis of thermal entanglement is that, although standard statistical physics is characterized by the partition function, determined by only the eigenvalues of the system, thermal entanglement properties require in addition knowledge of the eigenstates. In other words thermal entanglement is determined by both eigenstates and eigenvalues of the density operator $\rho(T)$. An interesting behavior of the thermal entanglement is that it can increase with the increase of temperature and magnetic fields [9,10]. A natural question is if we can induce the violation of Bell inequality and the violation of reduction criteria [5] by changing temperature and magnetic fields.

Arnesen *et al.* [9] pointed out that one can test the Clauser-Horne-Shimony-Holt (CHSH) inequality [18,19] for the thermal state by measuring different components of the magnetic susceptibility tensor since the different components of the magnetic susceptibility tensor are proportional to spin-spin correlations in different pairs of directions. Very recently Mancini and Bose [20] proposed a scheme for producing robust thermal entanglement between atoms in distant cavities connected by an optical fiber, and the scheme serves as an experiment to detect thermal entanglement when the cavities are very near.

In this paper we will study the violation of Bell inequality and reduction criteria for thermal states of qubits which interact via a multi-qubit Heisenberg interaction model. One particular case of this model was recently realized in cavity-QED by Zheng [21]. We will also discuss the violations in this realistic model.

The most commonly discussed Bell-inequality is the CHSH inequality. The CHSH operator ($\vec{a}, \vec{a}', \vec{b}, \vec{b}'$ are unit vectors) reads

$$\hat{B} = \vec{a} \cdot \vec{\sigma} \otimes (\vec{b} + \vec{b}') \cdot \vec{\sigma} + \vec{a}' \cdot \vec{\sigma} \otimes (\vec{b} - \vec{b}') \cdot \vec{\sigma}. \quad (2)$$

In the above notation, the Bell inequality reads

$$|\langle \hat{B} \rangle| = |\text{tr}(\rho \hat{B})| \leq 2, \quad (3)$$

where ρ is an arbitrary two-qubit state. The maximal amount of Bell violation of a state ρ is given by [22]

$$\mathcal{B} = 2\sqrt{u + \tilde{u}}, \quad (4)$$

where u and \tilde{u} are the two largest eigenvalues of $T_\rho T_\rho^\dagger$, T_ρ being the 3×3 matrix whose elements is

$$(T_\rho T_\rho^\dagger)_{nm} = \text{tr}(\rho \sigma_n \otimes \sigma_m). \quad (5)$$

Here $\sigma_1 \equiv \sigma_x$, $\sigma_2 \equiv \sigma_y$, and $\sigma_3 \equiv \sigma_z$ are the usual Pauli matrices.

Now we define a quantity

$$M = u + \tilde{u} - 1 \quad (6)$$

which ranges from -1 to 1. The quantity M , which we call *violation measure* of Bell inequality in this paper, indicates the Bell violation when $M > 0$ and maximal Bell violation when $M = 1$.

For any pure and some special mixed two-qubit state, there exists a simple relation [23] between the concurrence [24] C (the measure of entanglement) and the maximal violation of the Bell inequality:

$$\mathcal{B} = 2\sqrt{1 + C^2}. \quad (7)$$

We see from the above equation that the entanglement implies the violation of Bell inequality. But for a general mixed state, there is no this simple relation.

We consider a N -qubit Heisenberg model

$$H = \frac{J}{4} \sum_{i \neq j}^N (\sigma_{ix} \otimes \sigma_{jx} + \sigma_{iy} \otimes \sigma_{jy} + \Delta \sigma_{iz} \otimes \sigma_{jz}) + \frac{B}{2} \sum_{i=1}^N \sigma_{iz}, \quad (8)$$

where J is the exchange coupling constant, Δ is the anisotropic parameter, and B is the magnetic field along z direction. In this model all particles interact equally with each other. The model reduces to the two-qubit model for $N = 2$ and to the three-qubit Heisenberg model with the periodic boundary condition for $N = 3$, respectively.

By using the collective spin operators $S_\alpha = \sum_{i=1}^N \sigma_{i\alpha}/2$ ($\alpha = x, y, z$), the Hamiltonian is rewritten as

$$H = J(S_x^2 + S_y^2 + \Delta S_z^2) + BS_z = J\tilde{S}^2 + J(\Delta - 1)S_z^2 + BS_z \quad (9)$$

up to a trivial constant. Due to the key term S_z^2 one can generate multipartite maximally entangled states in this system [25,21]

The partition function is obtained as [11]

$$Z = \sum_{k=0}^{N/2} N_k \sum_{m=0}^{N-2k} e^{-\beta J[(\Delta-1)(m-N/2+k)^2]} e^{-\beta B(m-N/2+k)} \times e^{-\beta J(N/2-k)(N/2-k+1)}, \quad (10)$$

where $N_k = \binom{N}{k} - \binom{N}{k-1}$ and $\binom{N}{-1} = 0$.

The reduced density matrix for any two qubits is given by [11]

$$\rho_{12} = \frac{1}{4} [1 + (v_+ - v_-)(\sigma_{1z} + \sigma_{2z}) + 2y(\sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y}) + (1 - 4w)\sigma_{1z}\sigma_{2z}] \quad (11)$$

with matrix elements

$$v_\pm = \frac{N^2 - 2N + 4\langle S_z^2 \rangle \pm 4\langle S_z \rangle(N-1)}{4N(N-1)},$$

$$w = \frac{N^2 - 4\langle S_z^2 \rangle}{4N(N-1)},$$

$$y = \frac{2\langle S_x^2 + S_y^2 \rangle - N}{2N(N-1)}. \quad (12)$$

The relevant expectation values are given by [11]

$$\langle f(S_z) \rangle = \sum_{k=0}^{N/2} N_k \sum_{m=0}^{N-2k} f(m - N/2 + k) \times e^{-\beta J[(\Delta-1)(m-N/2+k)^2]} e^{-\beta B(m-N/2+k)} \times e^{-\beta J(N/2-k)(N/2-k+1)} / Z,$$

$$\langle S_x^2 + S_y^2 \rangle = \sum_{k=0}^{N/2} N_k \sum_{m=0}^{N-2k} [(N/2 - k)(N/2 - k + 1) - (m - N/2 + k)^2] \times e^{-\beta J[(\Delta-1)(m-N/2+k)^2]} e^{-\beta B(m-N/2+k)} \times e^{-\beta J(N/2-k)(N/2-k+1)} / Z. \quad (13)$$

Here $f(S_z)$ is an arbitrary function of S_z . Eqs.(10)–(13) gives completely the reduced density matrix. Along the standard procedures for calculating the maximal violation and the concurrence, they are obtained as

$$M \equiv M(J, \Delta, \beta, B) = 8y^2 + (1 - 4w)^2 - \min[4y^2, (1 - 4w)^2] - 1 \quad (14)$$

$$C \equiv C(J, \Delta, \beta, B) = 2 \max\{0, |y| - \sqrt{v_+ v_-}\} \quad (15)$$

For $N = 2$, Eqs.(14) and (15) become

$$M = \{2 \sinh^2(\beta J) + [\cosh(\beta B) e^{-\beta \Delta J} - \cosh(\beta J)]^2 - \min\{\sinh^2(\beta J), [\cosh(\beta B) e^{-\beta \Delta J} - \cosh(\beta J)]^2\} / [\cosh(\beta B) e^{-\beta \Delta J} + \cosh(\beta J)]^2 - 1, \quad (16)$$

$$C = \max\{0, \sinh(\beta |J|) - e^{-\beta \Delta J} / [\cosh(\beta B) e^{-\beta \Delta J} + \cosh(\beta J)]\}. \quad (17)$$

From the analytical expressions of M and C we immediately obtain

$$M(J, \Delta, \beta, B) = M(-J, -\Delta, \beta, B),$$

$$C(J, \Delta, \beta, B) = C(-J, -\Delta, \beta, B), \quad (18)$$

$$M(J, \Delta, \beta, B) = M(J, \Delta, \beta, -B),$$

$$C(J, \Delta, \beta, B) = C(J, \Delta, \beta, -B). \quad (19)$$

From Eq.(18) we see that the violation of Bell inequality is invariant under the simultaneous sign changes of the parameters Δ and J . The entanglement also has the same property. In particular the violation does not depend on the sign of J when $\Delta = 0$ which implies that the violations are same for the antiferromagnetic ($J > 0$) and ferromagnetic cases ($J < 0$) in the XX model. From Eq.(19) we know that M are symmetric with respect to B . Although this conclusion is obtained for the case of $N = 2$, it is valid for any N in our model.

Fig.1 gives numerical calculations of the violation measure and concurrence as a function of temperature for different magnetic fields. The concurrence is plotted in this paper for a comparison. It is clear from Fig.1 that there exist critical temperatures T_M (T_C) for the violation measure (the entanglement). After the critical temperature T_M (T_C) the Bell inequality is not violated (the entanglement disappears). Note that T_C is independent on the magnetic fields, while T_M decreases with the increase of magnetic fields. We also observe that $T_M < T_C$ which implies the fact that some entangled states do not violate a Bell inequality. In the temperature range $T_M < T < T_C$, the state is entangled but the Bell inequality is not violated. Now we see the case of $B = 2.5$. The entanglement can be increased by increasing the temperature, however the Bell inequality is not violated at any temperatures. The comparison shows that the behavior of the violation measure is very different from that of the concurrence.

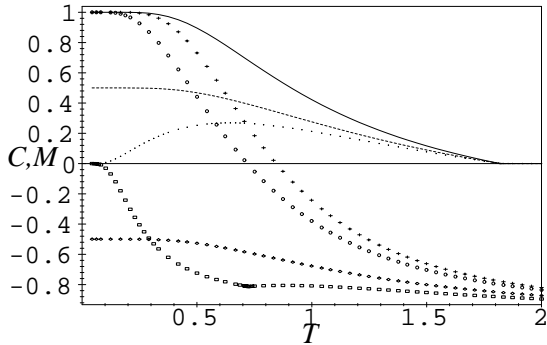


FIG. 1. The violation measure and the concurrence as a function of temperature for different magnetic fields. Violation measure: $B = 0$ (cross points), $B = 1$ (circle points), $B = 2$ (diamond points) and $B = 2.5$ (box points); The concurrence: $B = 0$ (solid line), $B = 2$ (dashed line), and $B = 2.5$ (dotted line). The parameters $J = \Delta = 1$ and $N = 2$.

In Fig.2 we plot the violation measure as function of temperature for different number of qubits. The results

show that although we can have entanglement the Bell inequality can not be violated for $N \geq 3$. Then we see if the magnetic fields can induce the violation for $N \geq 3$. The violation measure versus the magnetic field is given in Fig. 3. The temperature is choose to be close to the absolute zero temperature. From Fig.3 we see that we still can not obtain the violation of Bell inequality for $N \geq 3$ by increasing the magnetic fields although the entanglement can be increased by the magnetic fields. For the case of $N = 2$ we find the critical magnetic field B_M for the violation measure and B_C for the concurrence. The critical magnetic field B_M is less than B_C .

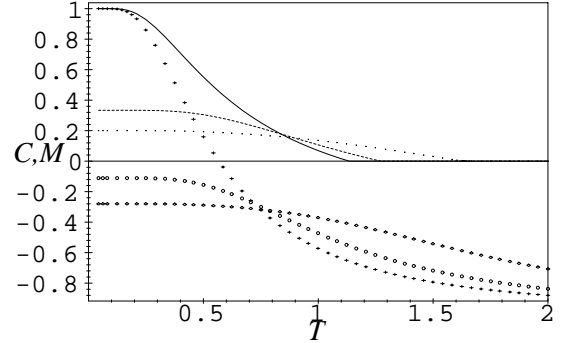


FIG. 2. The violation measure and the concurrence as a function of temperature for different number of qubits. The violation measure: $N = 2$ (cross points), $N = 3$ (circle points), and $N = 5$ (diamond points); The concurrence: $N = 2$ (solid line), $N = 3$ (dashed line), and $N = 5$ (dotted line). The parameters $J = -1$ and $B = \Delta = 0$.

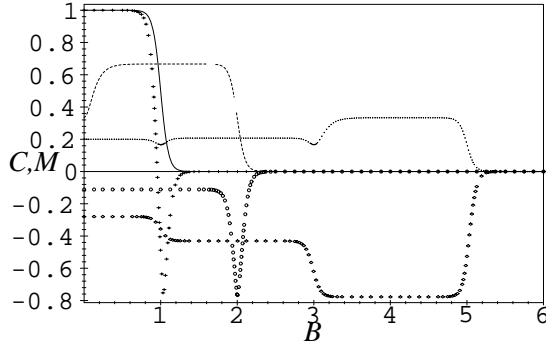


FIG. 3. The violation measure and the concurrence as a function of the magnetic field for different number of qubits. The violation measure: $N = 2$ (cross points), $N = 3$ (circle points), and $N = 6$ (diamond points); The concurrence: $N = 2$ (solid line), $N = 3$ (dashed line), and $N = 6$ (dotted line). The parameters $J = -1$, $T = 0.05$, and $\Delta = 0$.

Another interesting feature of quantum entanglement is that a bipartite entangled state (systems A and B) can be more disordered locally than globally [26]. If we measure the disorder by von Neumann entropy $S(\rho) = -\text{tr}(\rho \log_2 \rho)$, one inequality holds for all separable states

$$S(A), S(B) \leq S(A, B). \quad (20)$$

which is called reduction criterion [5]. For the models we are considering, $S(A) = S(B)$ holds. Then we define a quantity

$$R = S(A) - S(A, B), \quad (21)$$

which can be larger than zero and acts as a quantitative measure of the violation of the reduction criterion (20). The violation ($R > 0$) implies that the state is entangled.

From Eq.(11), the violation measure R is obtained as

$$R = v_+ \log_2 v_+ + v_- \log_2 v_- + (w - y) \log_2 (w - y) + (w + y) \log_2 (w + y) - (v_+ + w) \log_2 (v_+ + w) - (v_- + w) \log_2 (v_- + w). \quad (22)$$

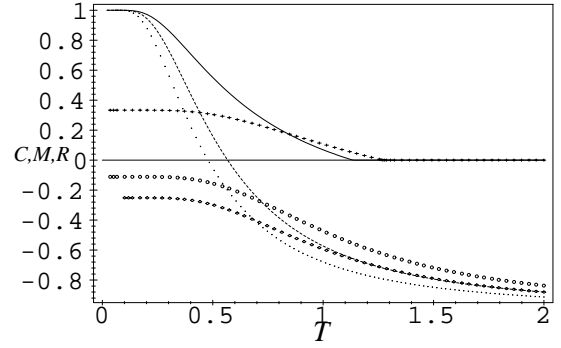


FIG. 4. The violation measure R of reduction criteria, the concurrence C and violation measure M as a function of T . We plotted C (solid line), M (dashed line), and R (dotted line) for $N = 2$ and C (cross points), M (circle points), and R (diamond points) for $N = 3$, respectively. The parameters $J = -1$ and $B = \Delta = 0$.

The numerical results are given in Fig.4. We find that the behaviors of the violation measures are similar. For $N = 2$, both the reduction criteria and Bell inequality can be violated. But the critical temperature T_R of the violation measure is different from T_M and T_C , i.e., $T_R < T_M < T_C$. There exists a temperature range $T_R < T < T_M$ in which the Bell inequality is violated while the reduction criteria is not violated. For $N = 3$ we still can not find any violation of both the reduction criteria and Bell inequality although the state is entangled for a range of temperature.

Finally we consider a realistic model in cavity QED. Consider the interaction of N qubits with a single cavity mode in the vacuum state via Tavis-Cummings model [27]. For the case of large detuning δ between qubits and the field mode, the effective Hamiltonian is given by [21]

$$H_e = \lambda(S_x^2 + S_y^2 + S_z), \quad (23)$$

where $\lambda = g^2/\delta$ and g is the atom-cavity coupling strength. Comparing Eqs.(23) and (8) we find $\Delta = 0$ and $J = B = \lambda$. Note that λ can be negative due to the detuning. The numerical results are shown in Fig.5. We see that the entanglement can be obtained while the Bell inequality and reduction criteria can not be violated.

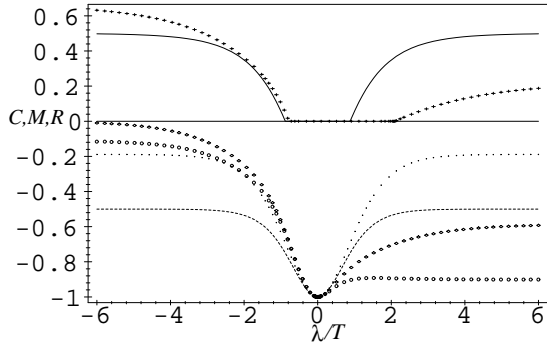


FIG. 5. The violation measures and the concurrence as a function of λ/T . We plotted C (solid line), M (dashed line), and R (dotted line) for $N = 2$ and C (cross points), M (circle points), and R (diamond points) for $N = 3$, respectively.

In conclusion we have studied the violation of Bell inequality and reduction criteria in the multi-qubit Heisenberg model. The results show that the the Bell inequality and the reduction criteria are violated for the case of $N = 2$ but not violated for the case of $N \geq 3$ at any temperature and magnetic fields in our model. Unlike the behaviors of the entanglement, the violations can not be induced by increasing temperature and magnetic fields. In comparison with the thermal entanglement, they are relatively hard to be obtained.

ACKNOWLEDGMENTS

The author thanks Klaus Mølmer, Hongchen Fu, Alan I Solomon, Ujjwal Sen, Mang Feng, R. de la Madrid, Barry C Sanders and Paolo Zanardi for helpful discussions. This work has been supported by the European Community through grant ISI-1999-10596 (Q-ACTA).

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